

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.93	22.5	0.93	22.1	0.93	22.1

Model Results

Predicted value: 362 °C

Global applicability domain: Outside

Local applicability domain index: 4.38e-01

Confidence level: 5.55e-01

Nearest Neighbors from the Training Set

Image not found

3,3'-Dimethylbenzidine

Measured: 339

Predicted: 371

Image not found

4,4'-Methylenedianiline

Measured: 398

Predicted: 368

Image not found

2,4'-Biphenyldiamine

Measured: 363

Predicted: 367

Image not found

Benzidine

Measured: 401

Predicted: 367

Image not found

1,2-Benzenediamine,N-phenyl-

Measured: 313

Predicted: 363